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A novel approach to quantum transport in coupled electron-phonon sytems has been developed. Application to the polaron problem, two-level systems and semiconductor double-well structures has been made. We find that dissipative effects in the electronic system can be obtained. Furthermore, a theoretical model for the electronic density of states for (imperfect) semiconductor systems has been developed to aid interpretation of transport data. This model has been successfully applied to ternary alloys, as well as amorphous semiconductor quantum wells.

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Theory of Transport for Interacting Many-Body Systems

Final Report

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Introduction

The research effort covered by this grant has been concentrated on two aspects of quantum transport theory: development and application of a general and manageable formalism suitable for transport in mesoscopic systems and an efficient model to account for the electronic structure of semiconductor heterostructures and alloys. The latter is important to aid interpretation of transport measurements in narrow semiconductor quantum well structures, both from crystalline and amorphous materials.

(A) Development of a New Approach to the Theory of Quantum Transport

A coherent–state functional integral approach has been developed to describe general coupled fermion–boson systems in thermal equilibrium, as well as under the influence of an external field of *arbitrary strength*. Our approach, while extremely general, has been developed with charge transport in solids kept in mind. In this context, our formalism accounts for a situation where one is primarily interested in the behavior of the fermionic charge carriers. The phonon system is of merely indirect importance, although, it has a profound influence on the behavior of the former. We have considered a situation where the electron–phonon system originally is in thermal equilibrium with an unspecified bath, characterized by temperature and chemical potential. At some point in time (t=0), an external field is applied and drives the system out of equilibrium. Such a situation is standard in the physics of electronic devices but applies to a variety of physical situations. As the primary interest is devoted to the electrons, it is desirable to eliminate the phonon degrees of freedom. This is possible analytically for the important class of the electron–phonon interaction which is linear in the ion displacement. The coupled electron system may subsequently be treated by many–body techniques and described in terms of an expansion series around a mean–field approximation.

The general formalism, including the mean–field equations and higher–order correction terms, has been developed. Within lowest order of approximation we find that the interacting electron system can be described by generalized (time–dependent) mean–field equations which account for both the electron–electron and electron–phonon coupling. In thermal equilibrium, the electron–phonon interaction leads to quantitative changes in the properties of the system, essentially contained in a renormalization of the one–particle energies. Out of thermal equilibrium, qualitative differences occur in the time–evolution of the system due to the non–Markovian nature of the electron–phonon terms. In general, they give rise to irreversible ("dissipative") behavior of the electron system.

In the language of density matrices, the lowest order approximation provides a reduced one–particle density matrix which is diagonal in the self–consistently calculated solutions of the mean–field equations. Higher–order correction terms provide off-diagonal contributions.

We have applied this approach to several (model) systems. First, we considered thermal equilibrium of an independent–boson system and found that our lowest–order approximation, indeed, gives the exact result for the most simple model cases.[1] Moreover, we found

that when applied to the ground state (T=0) of a single polaron problem, our lowest order approximation is identical to the adiabatic approximation which has been developed by Pekar and Deigen, [2] and is based on a variational calculation. Advantage of our formalism, however, is the fact that it provides well defined correction terms. We are presently performing a numerical study of the single polaron and hope to be able to extend this study to bi-polarons in the very near future.

Other applications concerned themselves with two-level systems coupled to a phonon bath. In particular, we considered a system where the electron-phonon coupling influences the inter-level coupling. We have been able to show that our simple model indeed gives rise to a "destruction of phase coherence", i.e., a damping of the Rabi oscillations, where expected on physical grounds. [3] Moreover, we used a more realistic model system and acoustic phonons to study coherent charge oscillations in semiconductor double wells. [4] Within some simplifying assumptions we have shown that this system may be described by a two-level system. Again, we find that, for a wide parameter range, phonon emission and absorption processes lead to a loss of phase coherence. At this point, however, the latter study must be considered preliminary because important effects, such as the carrier-carrier interaction and possible inhomogeneities within a quantum well, have not been included. Nevertheless, these studies have indicated that, in spite of its relative simplicity and numerical tractability, complex many-body problems may be treated within this formalism. Therefore, more numerically demanding applications to more realistic situations, such as charge transport in resonant-tunneling systems, is planned.

There also remain a few open questions concerning this approach. The stationary-phase approximation, which underlies this approximation scheme is, strictly speaking, not justified in terms of a large expansion parameter. However, it gives physically intuitive results. The ultimate test for the validity of a mean-field approximation lies in the successful application to physical systems. One of the striking features of the approximation is that the phonon temperature (e.g., in form of the Planck distribution function) does not enter the time-evolution of the system in lowest order. Closer inspection shows, that the spontaneous emission term cancels the absorption term in the effective phonon potential term. To what extent this requires the inclusion of higher-order terms which arise from the SPA is yet unclear.

Another, from a physical standpoint, yet unresolved issue is the finding that, for wide barriers, the charge oscillations between barriers are not damped by acoustic phonons. The phonon term is a time convolution between a phonon-dependent term and an electronic term. If the frequencies which characterize these two functions are rather different from each other, the efficiency of the phonon term is small. Again. phonon-emission and absorption processes seem to largely compensate each other "coherently".

Rather recently, we have shown that the present formalism may also be applied, in rather similar fashion, to spin systems explicitly coupled to phonons. Introducing Schwinger bosons to describe the spin degrees of freedom, the problem can be viewed as a coupled system of three types of bosons. The same technical steps in the manipulation of the statistical averages lead to similar mean-field equations as in the transport case. Again, in thermal equilibrium,

system characteristics are renormalized whereas, for the time-evolution, non-Markovian behavior is found. Different forms of mean-field equations may be obtained depending on the pairing scheme of boson fields.[5] A more detailed study of spin systems is planned in the near future.

(B) Electronic Structure of Disordered Semiconductors

In an attempt to shed light on transport properties in disordered semiconductors, we have developed a very efficient and versatile cluster model for the electronic density of states. The electronic structure, next to the nature of the electron–phonon interaction, has an important influence on the transport properties of the system. Our approach is based on a large cluster calculation based on a tight–binding model. Lattice mismatch in the constituent materials may lead to local bond–length and angle fluctuations. These are accounted for by an efficient Keating–type potential. Our model is applicable to virtually every semiconductor alloy which is presently considered for device application, as well as a variety of more complex non–periodic semiconductor structures.

Our main findings for $Al_xGa_{1-x}As$ and $ZnTe_xSe_{1-x}$ have been presented in detail in a previous report.[6,7,8] In summary, *quantitative* agreement with experiment has been achieved for the first time for these alloys. Starting from exclusively bulk properties of the constituent materials, as well as the band offset, we have been able to quantitatively explain the composition dependence of the main energy gap. We find that pure substitutional disorder accounts for all/most of the discrepancy between results from the virtual crystal approximation and experiment. For alloys from lattice–mismatched constituents, such as $ZnTe_xSe_{1-x}$, we find that bond–angle fluctuations also play an important role in narrowing the main energy gap. Bond–length variations are small and have practically no effect on the width of the main energy.

Recently, we have obtained first results for a study of a–Si quantum wells provided by Si–C barrier layers. We have constructed a simplified model for an amorphous semiconductor quantum well. Starting from a 30000 atom cluster of crystalline Si, a continuous random network of amorphous Si (a–Si) was created by elementary bond switching and subsequent annealing. The interface between a–Si and c–Si was relaxed continuously to release elastic strain. Finally, every other Si atom in the crystalline part of the cluster was replaced by a C atom. The latter simply consisted in replacing Si tight–binding parameters by C parameters corresponding to silicon carbide. This procedure avoids a detailed modeling of the interface between two amorphous systems which can be expected to contain a large number of defects and impurities, such as hydrogen, to accommodate lattice mismatch. For layers as narrow as 2nm and less, our studies of this model system reveal clear evidence for confinement effects in form of a certain widening of the main energy gap and the formation of steps, indicating the formation of a 2d density of states. These features are evident when averaging over a large number (≥ 30) of sites which are picked at random within the center sheet of the well. As expected these features are less pronounced than in crystalline materials, but clearly resolvable nonetheless. Secondly, we find that the local density of states is rather site dependent. Studying neighboring sites, we find that *local* confinement effects are present for narrow layers and are strongly site–dependent. Therefore, the confinement effects observed in amorphous semiconductors can not be viewed as the formation of "subbands", as in case of crystalline materials. Our findings give strong theoretical support to indirect conclusions from transport measurements.[9]

As confinement effects are most pronounced in narrow layers, details of the interfaces

may influence the density of states and confinement effects. To investigate this issue, we plan to construct a different cluster, in which the lattice mismatch across the interface is accommodated by defects, such as dangling bonds and hydrogen incorporation.

LIST OF PUBLICATIONS AND TECHNICAL REPORTS SUPPORTED UNDER THIS GRANT

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